

D-Phenylalanine
673-06-3 | DTXSID4025876

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.68e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.05e-01

Confidence level: 4.32e-01

Nearest Neighbors from the Training Set

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N,N-Dimethylformamide

Measured: 8.20e-05

Predicted: 5.14

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4-Isopropylphenol

Measured: 1.92e-07

Predicted: 3.08e-02

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N-Methylaniline

Measured: 2.60e-02

Predicted: 2.12e-01

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Benzoic acid, 2-methoxy-

Measured: 2.89e-05

Predicted: 3.44e-04

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o-Vinyltoluene

Measured: 1.71e-05

Predicted: 1.93